CONTENTS

Special Issue: Applied Theoretical Chemistry 1990. Part III
Part I was published in J. Mol. Struct. (Theochem), 230
Part II was published in J. Mol. Struct. (Theochem), 232

Decomposition of electron density matrix and total energy of supermolecule in the method of non-orthogonal localized molecular orbitals
S.A. Egupov (Kharkov, USSR) 1
Analytical formulae for the enumeration of substitutional isomers of planar molecules
Yu.A. Kruglyak and M.E. Dochtmanov (Odessa, USSR) 13
On graph theoretical SAR and the mathematical theory of categories
S.C. Grossman (Omaha, NE, USA) 21
Halogen effects on the electronic characteristics of C=C, N=C and P=C bonds
V.I. Kharchenko and L.N. Alexeiko (Vladivostok, USSR), V.V. Penkovsky (Kiev, USSR), S.A. Pavlenko and A.V. Kashin (Vladivostok, USSR) 35
Correlation of enthalpy of octanes with orthogonal connectivity indices
M. Randić (Des Moines, IA, USA) 45
Applications of the many-body perturbation theory in the localized representation: structural effects in the correlation energy of normal saturated hydrocarbons
E. Kapuy, F. Bogár and F. Bartha (Szeged, Hungary) and C. Kozmutza (Budapest, Hungary) 61
Studies on electronegativity equalization. Part 1. Consistent diatomic partial charges
L. von Szentpály (Kingston, Jamaica) 71
Substituent effects on carbonyl bond orders
S. Ranganathan (New Delhi, India) 83
Manifestations of stability interplay between potential-hypersurface multiple energy minima in heat-capacity enhancement
Z. Slanina (Mainz, Germany) 89
Molecular orbital theory on straight chain conjugate polymers
Z.Z. Yang (Changchun, People's Republic of China) 99
Computational test for the performance of the improved MM2 aromatic force field
P.M. Ivanov and T.G. Momchilova (Sofia, Bulgaria) 115
Multiconfiguration self-consistent-field (MCSCF) approaches to organic structures and reactivities
H.T. Yu and J.D. Goddard (Guelph, Ont., Canada) 129
Interaction energy of formaldehyde with ammonia
C. Kozmutza, (Budapest, Hungary), E.M. Evleth (Paris, France) and E. Kapuy (Budapest, Hungary) 139
Conformational potential energy curves for low lying excited states of selected polyfluorobiphenyl (PFB) and polychlorobiphenyl (PCB) congeners
T.-H. Tang, M. Nowakowska, J.E. Guillet and I.G. Csizmadia (Toronto, Ont., Canada) 147
Protonation and hydration of hydroxyketene
J. Andraos and A.J. Kresge (Toronto, Ont., Canada) 165
A refined theoretical investigation of the oxygen-electrode processes of an alkaline hydrogen–oxygen fuel cell
T.-H. Tang, I.G. Csizmadia, L. Pataki, R.D. Venter and C.A. Ward (Toronto, Ont., Canada) 185
Free-energy relationships in organic electron transfer reactions
L.G. Arnaut and S.J. Formosinho (Coimbra, Portugal) 209
Ab initio study of C_6H_7 radicals involved in the photolyses of 3-methylcyclopentene and 3-methyl-1,4-pentadiene
G.R. De Maré (Brussels, Belgium) and G.J. Collin (Chicoutimi, Que., Canada) 231
Specificity of transcription and incorporation of nucleoside analogues
R.P. Ojha, M. Roychoudhury and N.K. Sanyal (Gorakhpur, India) 247

Biological activity of 7-deazaadenine nucleoside antibiotics: a theoretical study
R.P. Ojha and N.K. Sanyal (Gorakhpur, India) 275
Theoretical conformational analysis, electronic structure and molecular modelling studies in dihydropteroate synthase inhibition by multisubstituted sulphones
Yu.A. Sokolov (Minsk, USSR), M.C. Menziani, M. Cocchi and P.G. De Benedetti (Modena, Italy) 293
Molecular orbital studies on β-blockers: conformation of acetophenone-*O*-(*tert*-butylamino-3-hydroxy-2-propyl) oxime and (*tert*-butylamino-3-hydroxy-2-propylimino)-9-fluorene
A. Saran (Bombay, India) and R.P. Ojha (Gorakhpur, India) 301
Conformation of bioactive peptides: synthetic encephalins
A. Saran, M.M. Dhingra and Y.U. Sasidhar (Bombay, India) 315
Comparative study of the charge distribution in tetravalent carbonyl transients and organophosphorus adducts of trypsin
I.M. Kovach (Washington, DC, USA) and D. Huhta (Lawrence, KS, USA) 335
Molecular orbital study of the nitrogen basicity of prazosin analogues in relation to their α_1-adrenoceptor binding affinity
P.G. De Benedetti, M.C. Menziani, G. Rastelli and M. Cocchi (Modena, Italy) 343

Concluding Remarks 353

Author Index 357

Subject Index 359